



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:18 pm BST

PDB ID : 6LP5
Title : Structure of Sinonovacula constricta ferritin
Authors : Su, X.R.; Ming, T.H.; Su, C.
Deposited on : 2020-01-08
Resolution : 1.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

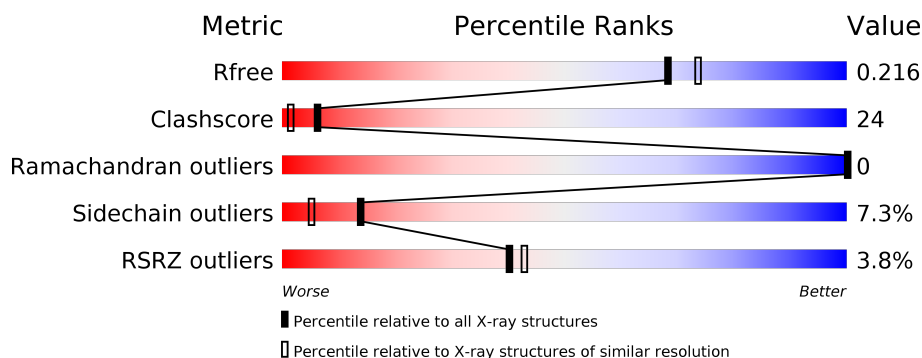
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	171	<div> <div>4%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>5%</div> <div>..</div> </div> </div>
1	B	171	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>5%</div> <div>..</div> </div> </div>
1	C	171	<div> <div>6%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>5%</div> <div>..</div> </div> </div>
1	D	171	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>5%</div> <div>..</div> </div> </div>
1	E	171	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> <div>..</div> </div> </div>
1	F	171	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>6%</div> <div>..</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9849 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	13	0
			1484	926	261	289	8			
1	B	170	Total	C	N	O	S	0	14	0
			1491	927	262	294	8			
1	C	170	Total	C	N	O	S	0	13	0
			1486	927	261	291	7			
1	D	170	Total	C	N	O	S	0	15	0
			1499	932	262	298	7			
1	E	170	Total	C	N	O	S	0	15	0
			1504	936	262	297	9			
1	F	170	Total	C	N	O	S	0	9	0
			1430	895	252	275	8			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by author).

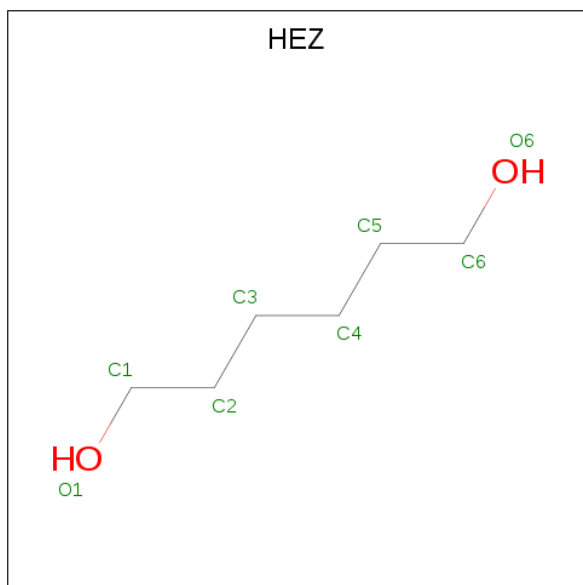
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Fe	0	0
			2	2		
3	E	2	Total	Fe	0	0
			2	2		
3	B	2	Total	Fe	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	2	Total	Fe	0	0
			2	2		
3	A	2	Total	Fe	0	0
			2	2		
3	F	2	Total	Fe	0	0
			2	2		

- Molecule 4 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		
4	C	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

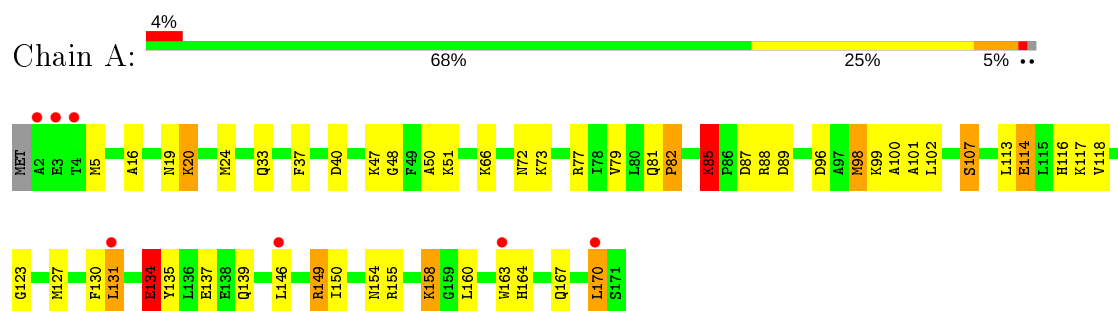
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total 152	O 152	0	0
5	B	139	Total 139	O 139	0	0
5	C	147	Total 147	O 147	0	0
5	D	153	Total 153	O 153	0	0
5	E	143	Total 143	O 143	0	0
5	F	151	Total 151	O 151	0	0

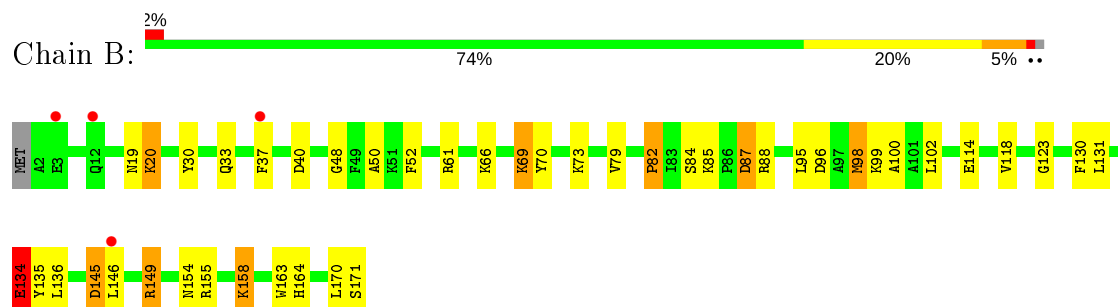
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

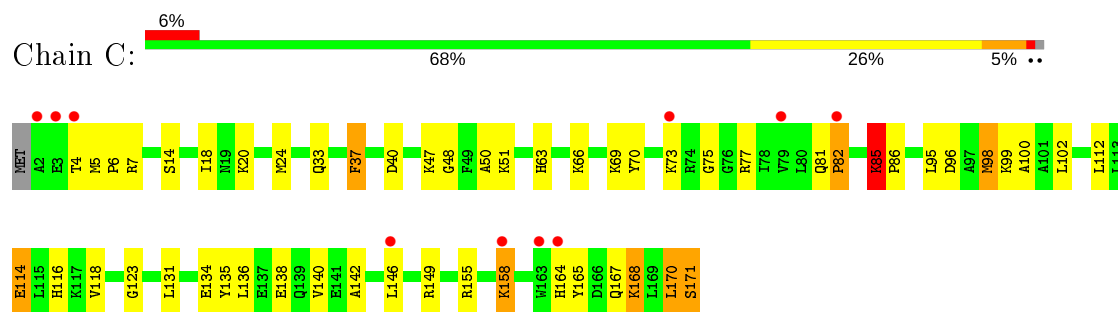
• Molecule 1: Ferritin



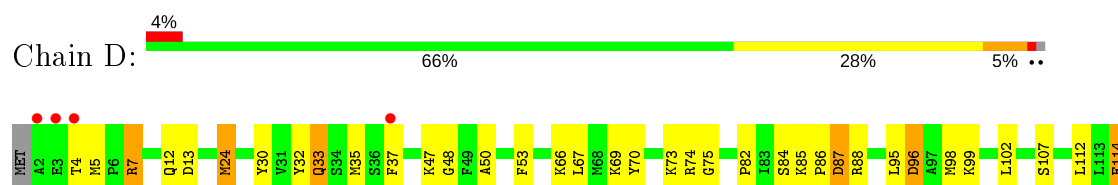
• Molecule 1: Ferritin



• Molecule 1: Ferritin

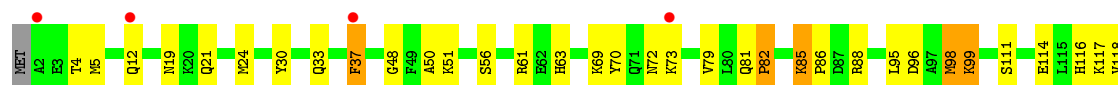


• Molecule 1: Ferritin





• Molecule 1: Ferritin



• Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	154.51Å 154.51Å 129.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.26 – 1.98 49.62 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (109.26-1.98) 99.9 (49.62-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.64 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.163 , 0.203 0.182 , 0.216	Depositor DCC
R_{free} test set	5243 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9849	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, FE, HEZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.16	5/1510 (0.3%)	1.09	14/2021 (0.7%)
1	B	1.08	5/1517 (0.3%)	1.04	10/2030 (0.5%)
1	C	1.16	3/1512 (0.2%)	1.13	11/2024 (0.5%)
1	D	1.13	2/1525 (0.1%)	1.19	15/2043 (0.7%)
1	E	1.08	3/1530 (0.2%)	1.09	9/2047 (0.4%)
1	F	1.20	9/1456 (0.6%)	1.09	11/1952 (0.6%)
All	All	1.13	27/9050 (0.3%)	1.11	70/12117 (0.6%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	114	GLU	CD-OE2	-7.29	1.17	1.25
1	E	134	GLU	CD-OE1	-7.17	1.17	1.25
1	B	84	SER	CB-OG	6.91	1.51	1.42
1	A	114	GLU	CD-OE1	-6.66	1.18	1.25
1	A	134	GLU	CD-OE2	-6.65	1.18	1.25
1	F	114	GLU	CG-CD	-6.55	1.42	1.51
1	D	84	SER	CB-OG	6.44	1.50	1.42
1	F	134	GLU	CD-OE2	-6.38	1.18	1.25
1	F	114	GLU	CB-CG	-6.25	1.40	1.52
1	F	114	GLU	CD-OE1	-6.21	1.18	1.25
1	C	114	GLU	CD-OE1	-6.07	1.19	1.25
1	B	134	GLU	CG-CD	-5.92	1.43	1.51
1	D	134	GLU	CD-OE1	-5.90	1.19	1.25
1	E	134	GLU	CG-CD	-5.74	1.43	1.51
1	B	134	GLU	CD-OE2	-5.59	1.19	1.25
1	B	87	ASP	CB-CG	5.47	1.63	1.51
1	C	114	GLU	CB-CG	-5.41	1.41	1.52
1	F	134	GLU	CG-CD	-5.27	1.44	1.51
1	B	134	GLU	CB-CG	-5.24	1.42	1.52
1	A	134	GLU	CG-CD	-5.23	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	72	ASN	CG-OD1	-5.22	1.12	1.24
1	F	134	GLU	CB-CG	-5.22	1.42	1.52
1	C	165	TYR	CZ-OH	-5.20	1.29	1.37
1	A	134	GLU	CB-CG	-5.18	1.42	1.52
1	E	134	GLU	CB-CG	-5.18	1.42	1.52
1	F	163	TRP	CB-CG	-5.13	1.41	1.50
1	A	72	ASN	CG-OD1	-5.03	1.12	1.24

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	MET	CG-SD-CE	-12.24	80.61	100.20
1	D	170	LEU	CB-CG-CD1	9.78	127.63	111.00
1	C	5	MET	CG-SD-CE	9.52	115.44	100.20
1	C	170	LEU	CB-CG-CD1	9.17	126.59	111.00
1	D	87[A]	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	D	87[B]	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	D	87[A]	ASP	CB-CG-OD1	8.96	126.36	118.30
1	D	87[B]	ASP	CB-CG-OD1	8.96	126.36	118.30
1	F	170	LEU	CB-CG-CD2	-8.43	96.66	111.00
1	D	149	ARG	CG-CD-NE	-8.42	94.11	111.80
1	E	85	LYS	CD-CE-NZ	7.88	129.81	111.70
1	C	98	MET	CG-SD-CE	-7.74	87.81	100.20
1	D	74	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	C	85	LYS	CD-CE-NZ	7.49	128.93	111.70
1	A	100	ALA	CB-CA-C	7.33	121.10	110.10
1	D	155	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	170	LEU	CB-CG-CD1	7.15	123.15	111.00
1	A	155	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	20	LYS	CD-CE-NZ	7.00	127.81	111.70
1	D	98	MET	CG-SD-CE	-6.95	89.08	100.20
1	E	98	MET	CG-SD-CE	-6.94	89.10	100.20
1	F	85	LYS	CD-CE-NZ	6.92	127.62	111.70
1	F	98	MET	CG-SD-CE	-6.92	89.12	100.20
1	C	170	LEU	CB-CG-CD2	-6.91	99.26	111.00
1	F	96	ASP	CB-CG-OD2	6.80	124.42	118.30
1	E	117	LYS	CD-CE-NZ	6.76	127.26	111.70
1	B	100	ALA	CB-CA-C	6.63	120.04	110.10
1	D	7	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	155	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	E	37	PHE	CB-CA-C	6.56	123.52	110.40
1	E	148	ASP	CB-CG-OD1	6.48	124.13	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	87	ASP	CB-CG-OD1	6.48	124.13	118.30
1	F	89	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	C	37	PHE	CB-CA-C	6.39	123.19	110.40
1	C	96	ASP	CB-CG-OD2	6.39	124.05	118.30
1	C	149	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	98	MET	CG-SD-CE	-6.28	90.15	100.20
1	F	170	LEU	CB-CG-CD1	6.25	121.62	111.00
1	A	98	MET	CG-SD-CE	-6.21	90.26	100.20
1	B	96	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	155	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	155	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	100	ALA	CB-CA-C	5.82	118.83	110.10
1	A	77	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	C	149	ARG	CG-CD-NE	-5.78	99.65	111.80
1	E	134	GLU	CB-CA-C	-5.76	98.89	110.40
1	A	96	ASP	CB-CG-OD2	5.72	123.45	118.30
1	D	134	GLU	CB-CA-C	-5.67	99.06	110.40
1	E	96	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	131[A]	LEU	CB-CG-CD1	5.63	120.57	111.00
1	A	131[B]	LEU	CB-CG-CD1	5.63	120.57	111.00
1	B	134	GLU	CB-CA-C	-5.63	99.15	110.40
1	D	96	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	155	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	85[A]	LYS	CD-CE-NZ	5.53	124.42	111.70
1	A	85[B]	LYS	CD-CE-NZ	5.53	124.42	111.70
1	B	87	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	5	MET	CG-SD-CE	5.48	108.96	100.20
1	D	170	LEU	CB-CG-CD2	-5.47	101.71	111.00
1	F	77	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	F	87	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	F	134	GLU	CB-CA-C	-5.34	99.71	110.40
1	E	61	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	77	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	74	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	149	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	134	GLU	CB-CA-C	-5.22	99.96	110.40
1	A	89	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	61	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	B	145	ASP	CB-CG-OD2	5.03	122.82	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1484	0	1416	85	0
1	B	1491	0	1409	57	0
1	C	1486	0	1427	70	0
1	D	1499	0	1420	66	0
1	E	1504	0	1429	71	0
1	F	1430	0	1356	100	0
2	A	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	B	8	0	14	4	0
4	C	8	0	14	3	0
4	D	8	0	14	3	0
4	E	16	0	28	3	0
4	F	16	0	27	2	0
5	A	152	0	0	20	1
5	B	139	0	0	12	0
5	C	147	0	0	13	0
5	D	153	0	0	16	0
5	E	143	0	0	20	1
5	F	151	0	0	17	0
All	All	9849	0	8554	429	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (429) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33[A]:GLN:OE1	1:A:37:PHE:CE2	1.63	1.48
1:B:33[B]:GLN:NE2	1:B:37:PHE:HE2	1.14	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33[A]:GLN:OE1	1:B:37:PHE:CE2	1.73	1.39
1:B:33[B]:GLN:NE2	1:B:37:PHE:CE2	1.94	1.33
1:F:33:GLN:OE1	1:F:37:PHE:CE2	1.82	1.32
1:F:171:SER:C	4:F:205:HEZ:O1	1.64	1.32
1:C:82:PRO:HD2	5:C:400:HOH:O	1.27	1.31
1:F:131[B]:LEU:O	1:F:131[B]:LEU:CD2	1.79	1.30
1:A:88[A]:ARG:NH2	5:A:301:HOH:O	1.64	1.28
1:F:82:PRO:HD2	5:F:392:HOH:O	1.15	1.28
1:B:82:PRO:HD2	5:B:391:HOH:O	1.12	1.26
1:E:82:PRO:HD2	5:E:396:HOH:O	1.08	1.25
1:F:33:GLN:OE1	1:F:37:PHE:HE2	0.91	1.24
1:F:131[B]:LEU:CD2	1:F:131[B]:LEU:C	1.99	1.21
1:B:33[A]:GLN:OE1	1:B:37:PHE:HE2	0.87	1.18
1:F:131[B]:LEU:HD22	1:F:131[B]:LEU:C	1.59	1.18
1:C:50:ALA:HB1	5:C:397:HOH:O	1.40	1.16
1:A:82:PRO:HD2	5:A:310:HOH:O	1.01	1.15
1:A:33[A]:GLN:OE1	1:A:37:PHE:HE2	0.83	1.15
1:E:142:ALA:HB2	5:E:328:HOH:O	0.95	1.13
1:F:131[B]:LEU:O	1:F:131[B]:LEU:HD23	1.38	1.13
1:B:50:ALA:HB1	5:B:379:HOH:O	1.48	1.11
1:A:149:ARG:HH11	1:A:149:ARG:CG	1.56	1.10
1:D:96:ASP:OD2	5:D:301:HOH:O	1.68	1.10
1:F:149:ARG:CG	1:F:149:ARG:HH11	1.63	1.10
1:A:116:HIS:HB2	1:A:131[B]:LEU:CD2	1.80	1.09
1:F:149:ARG:HG3	1:F:149:ARG:HH11	1.17	1.08
1:E:149:ARG:CG	1:E:149:ARG:HH11	1.63	1.06
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.17	1.06
1:C:131[B]:LEU:HD12	1:C:131[B]:LEU:O	1.52	1.06
1:D:50:ALA:HB1	5:D:391:HOH:O	1.55	1.06
1:F:50:ALA:HB1	5:F:397:HOH:O	1.53	1.05
1:A:116:HIS:HB2	1:A:131[B]:LEU:HD23	1.39	1.03
1:E:50:ALA:HB1	5:E:390:HOH:O	1.57	1.02
1:F:88[A]:ARG:HB3	1:F:88[A]:ARG:NH2	1.75	1.01
1:A:33[A]:GLN:CD	1:A:37:PHE:HE2	1.66	0.99
1:B:158:LYS:HD2	1:B:158:LYS:H	1.27	0.99
1:C:158:LYS:H	1:C:158:LYS:HZ3	1.08	0.98
1:E:95:LEU:HD11	1:E:99[B]:LYS:HE3	1.45	0.97
1:F:48:GLY:HA2	1:F:170:LEU:HD22	1.43	0.95
1:F:82:PRO:CD	5:F:392:HOH:O	1.83	0.94
1:E:149:ARG:HG2	1:E:149:ARG:HH11	1.29	0.94
1:B:171:SER:C	4:B:203:HEZ:H51	1.90	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33[B]:GLN:OE1	1:D:37:PHE:HE2	1.53	0.91
1:D:171:SER:C	4:D:203:HEZ:H22	1.93	0.89
1:A:51:LYS:HE3	1:A:170:LEU:HD22	1.55	0.88
1:A:149:ARG:NH1	1:A:149:ARG:CG	2.27	0.88
1:E:149:ARG:HH11	1:E:149:ARG:HG3	1.38	0.87
1:A:88[A]:ARG:NH1	5:A:304:HOH:O	2.07	0.87
1:A:51:LYS:HE3	1:A:170:LEU:CD2	2.03	0.87
1:A:88[B]:ARG:NH2	5:A:303:HOH:O	2.04	0.87
1:B:33[A]:GLN:CD	1:B:37:PHE:HE2	1.78	0.87
1:E:95:LEU:CD1	1:E:99[B]:LYS:HE3	2.03	0.87
1:B:20:LYS:HE2	5:B:393:HOH:O	1.73	0.87
1:C:158:LYS:H	1:C:158:LYS:NZ	1.73	0.86
1:A:158:LYS:CD	1:A:158:LYS:H	1.85	0.86
1:C:102:LEU:N	1:C:146[B]:LEU:HD21	1.91	0.86
1:A:146[B]:LEU:C	1:A:146[B]:LEU:HD23	1.97	0.85
1:F:149:ARG:HG3	1:F:149:ARG:NH1	1.84	0.85
1:D:107[A]:SER:OG	5:D:302:HOH:O	1.93	0.85
1:A:50:ALA:HB1	5:A:367:HOH:O	1.77	0.85
1:D:33[B]:GLN:OE1	1:D:37:PHE:CE2	2.29	0.85
1:A:20:LYS:HD3	5:A:313:HOH:O	1.78	0.84
1:D:99[A]:LYS:NZ	5:D:304:HOH:O	2.10	0.84
1:C:131[B]:LEU:C	1:C:131[B]:LEU:HD12	1.95	0.83
1:B:33[B]:GLN:HE21	1:B:37:PHE:HE2	0.88	0.83
1:C:82:PRO:HD3	1:E:85:LYS:HG2	1.61	0.82
1:F:69[B]:LYS:CG	5:F:421:HOH:O	2.28	0.82
1:A:149:ARG:HG3	1:A:149:ARG:HH11	1.41	0.82
1:A:118:VAL:HG22	5:A:425:HOH:O	1.79	0.82
1:F:48:GLY:HA2	1:F:170:LEU:CD2	2.10	0.81
1:F:102:LEU:N	1:F:146[B]:LEU:HD21	1.95	0.81
1:F:102:LEU:HA	1:F:146[B]:LEU:HD23	1.63	0.81
1:C:123:GLY:HA3	5:C:398:HOH:O	1.79	0.81
1:D:13:ASP:OD2	5:D:303:HOH:O	1.99	0.80
1:F:48:GLY:CA	1:F:170:LEU:CD2	2.60	0.80
1:A:33[A]:GLN:OE1	1:A:37:PHE:CZ	2.32	0.80
1:A:149:ARG:HG3	1:A:149:ARG:NH1	1.97	0.79
1:A:85[B]:LYS:HG2	1:B:82:PRO:HD3	1.66	0.78
1:F:149:ARG:HG2	1:F:149:ARG:HH11	1.48	0.78
1:A:164:HIS:NE2	1:C:164:HIS:CD2	2.52	0.78
1:F:131[B]:LEU:O	1:F:131[B]:LEU:HD22	1.61	0.78
1:A:123:GLY:HA3	5:A:384:HOH:O	1.83	0.78
1:B:33[B]:GLN:NE2	1:B:37:PHE:CZ	2.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:HIS:CB	1:A:131[B]:LEU:HD23	2.14	0.77
1:D:33[A]:GLN:OE1	1:D:37:PHE:HE2	1.68	0.76
1:F:11:HIS:CE1	1:F:12:GLN:HE22	2.02	0.76
1:C:146[B]:LEU:HD12	1:C:146[B]:LEU:O	1.84	0.76
1:A:137:GLU:OE1	5:A:302:HOH:O	2.02	0.76
1:D:87[B]:ASP:C	1:D:88[B]:ARG:HD2	2.06	0.76
1:D:96:ASP:CG	5:D:301:HOH:O	2.14	0.76
1:F:66:LYS:HD3	1:F:134:GLU:HG2	1.68	0.76
1:B:158:LYS:H	1:B:158:LYS:CD	1.91	0.75
1:E:171:SER:C	4:E:204:HEZ:C6	2.54	0.75
1:F:154:ASN:ND2	5:F:301:HOH:O	2.12	0.74
1:F:88[A]:ARG:HB3	1:F:88[A]:ARG:HH21	1.49	0.74
1:E:131[B]:LEU:HD12	1:E:131[B]:LEU:O	1.87	0.74
1:C:4:THR:HG21	1:C:75:GLY:O	1.88	0.73
1:C:158:LYS:HZ3	1:C:158:LYS:N	1.84	0.73
1:C:158:LYS:H	1:C:158:LYS:CE	2.02	0.72
1:E:171:SER:C	4:E:204:HEZ:H61	2.10	0.72
1:B:88[B]:ARG:HG3	1:B:88[B]:ARG:HH11	1.53	0.72
1:F:102:LEU:CA	1:F:146[B]:LEU:CD2	2.67	0.71
5:D:412:HOH:O	1:F:69[A]:LYS:CG	2.37	0.71
1:F:88[B]:ARG:HH11	1:F:91:TRP:HE3	1.38	0.71
1:B:123:GLY:HA3	5:B:360:HOH:O	1.90	0.71
1:F:4:THR:HG21	1:F:75:GLY:O	1.90	0.71
1:F:88[A]:ARG:HB3	1:F:88[A]:ARG:CZ	2.12	0.71
1:F:99[A]:LYS:HB2	1:F:99[A]:LYS:NZ	2.05	0.71
1:E:37:PHE:CD1	5:E:414:HOH:O	2.44	0.70
1:A:20:LYS:CD	5:A:313:HOH:O	2.37	0.70
1:E:149:ARG:HG3	1:E:149:ARG:NH1	1.99	0.70
1:E:82:PRO:CD	5:E:396:HOH:O	1.88	0.70
1:B:171:SER:C	4:B:203:HEZ:C5	2.59	0.70
1:D:4:THR:HG21	1:D:75:GLY:O	1.92	0.69
1:A:116:HIS:HB2	1:A:131[B]:LEU:HD21	1.73	0.69
1:A:149:ARG:HG2	1:A:149:ARG:NH1	1.97	0.69
1:B:88[B]:ARG:HG3	1:B:88[B]:ARG:NH1	2.06	0.68
1:E:137[A]:GLU:OE1	5:E:301:HOH:O	2.10	0.68
1:A:33[B]:GLN:O	1:A:37:PHE:HD2	1.77	0.68
1:B:130:PHE:O	1:B:134:GLU:HB2	1.93	0.68
1:E:123:GLY:HA3	5:E:381:HOH:O	1.93	0.68
1:E:21:GLN:NE2	1:E:24[B]:MET:CE	2.56	0.68
1:F:123:GLY:HA3	5:F:407:HOH:O	1.94	0.68
1:C:98:MET:SD	1:C:146[B]:LEU:HD13	2.33	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138[A]:GLU:OE2	5:C:301:HOH:O	2.11	0.68
1:A:130:PHE:O	1:A:134:GLU:HB2	1.95	0.67
1:B:70:TYR:HA	1:B:73[A]:LYS:HE3	1.77	0.67
1:C:82:PRO:HD3	1:E:85:LYS:CG	2.25	0.67
1:F:48:GLY:N	1:F:170:LEU:HD21	2.09	0.67
1:F:102:LEU:N	1:F:146[B]:LEU:CD2	2.58	0.67
1:C:123:GLY:CA	5:C:398:HOH:O	2.41	0.67
1:D:35:MET:CE	1:D:53:PHE:CE1	2.77	0.67
1:F:102:LEU:CA	1:F:146[B]:LEU:HD21	2.24	0.67
1:A:48:GLY:N	1:A:170:LEU:HD21	2.10	0.66
1:F:102:LEU:HA	1:F:146[B]:LEU:CD2	2.25	0.66
1:D:35:MET:HE3	1:D:53:PHE:CE1	2.31	0.66
1:E:63[B]:HIS:CE1	5:E:323:HOH:O	2.48	0.66
1:C:37:PHE:CD1	5:C:408:HOH:O	2.48	0.66
1:C:4:THR:HG22	1:C:7:ARG:HB2	1.78	0.66
1:D:130:PHE:O	1:D:134:GLU:HB2	1.95	0.66
1:D:158:LYS:CD	1:D:158:LYS:H	2.07	0.66
1:E:69:LYS:O	1:E:73[A]:LYS:HG3	1.95	0.65
1:B:145:ASP:OD2	1:B:149:ARG:NH1	2.29	0.65
1:A:158:LYS:HD3	1:A:158:LYS:H	1.59	0.65
1:C:66:LYS:HD3	1:C:134:GLU:HG2	1.77	0.65
1:E:142:ALA:CA	5:E:328:HOH:O	2.28	0.65
1:C:82:PRO:HD3	1:E:85:LYS:HB3	1.77	0.64
1:D:87[B]:ASP:O	1:D:88[B]:ARG:HD2	1.97	0.64
1:F:48:GLY:N	1:F:170:LEU:CD2	2.60	0.64
1:E:134:GLU:HB3	1:E:135:TYR:CD2	2.32	0.64
1:A:85[B]:LYS:CG	1:B:82:PRO:HD3	2.28	0.64
1:B:163:TRP:HZ2	5:B:416:HOH:O	1.81	0.64
1:D:131[B]:LEU:HD12	1:D:131[B]:LEU:O	1.98	0.63
1:D:154:ASN:ND2	5:D:305:HOH:O	2.25	0.63
1:F:128:CYS:SG	5:F:393:HOH:O	2.30	0.63
1:D:33[A]:GLN:OE1	1:D:37:PHE:CE2	2.50	0.63
1:E:116:HIS:HB2	1:E:131[B]:LEU:HD23	1.80	0.63
1:E:130:PHE:O	1:E:134:GLU:HB2	1.98	0.63
1:F:142:ALA:O	1:F:146[A]:LEU:HD13	1.99	0.63
1:D:66:LYS:HD3	1:D:134:GLU:CG	2.29	0.63
1:D:66:LYS:HD3	1:D:134:GLU:HG2	1.80	0.62
1:E:4:THR:HG22	5:E:405:HOH:O	1.98	0.62
1:D:128:CYS:SG	5:D:357:HOH:O	2.24	0.62
1:C:82:PRO:HD3	1:E:85:LYS:CB	2.29	0.62
1:D:158:LYS:H	1:D:158:LYS:HD2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LYS:O	1:D:73[A]:LYS:HG3	1.99	0.62
1:C:102:LEU:N	1:C:146[B]:LEU:CD2	2.62	0.62
1:D:134:GLU:HB3	1:D:135:TYR:CD2	2.35	0.62
1:C:69:LYS:O	1:C:73[A]:LYS:HG3	1.99	0.62
1:E:149:ARG:HG2	1:E:149:ARG:NH1	2.03	0.62
1:F:163:TRP:CH2	5:F:419:HOH:O	2.51	0.61
1:F:20:LYS:HD3	5:F:377:HOH:O	1.99	0.61
1:E:131[B]:LEU:HD12	1:E:131[B]:LEU:C	2.20	0.61
1:A:33[B]:GLN:O	1:A:37:PHE:CD2	2.52	0.61
1:D:171:SER:C	4:D:203:HEZ:C2	2.67	0.61
1:D:69:LYS:HG2	1:D:73[A]:LYS:HE2	1.83	0.61
1:F:99[A]:LYS:HB2	1:F:99[A]:LYS:HZ2	1.64	0.61
1:A:146[B]:LEU:HD23	1:A:146[B]:LEU:O	2.01	0.61
1:E:37:PHE:HD1	5:E:414:HOH:O	1.83	0.60
1:F:130:PHE:O	1:F:134:GLU:HB2	2.02	0.60
1:A:87:ASP:HB3	1:A:88[A]:ARG:HE	1.66	0.60
1:F:118:VAL:HG21	5:F:414:HOH:O	2.00	0.60
1:F:149:ARG:NH1	1:F:149:ARG:CG	2.32	0.60
1:C:33:GLN:OE1	1:C:37:PHE:CE2	2.54	0.60
1:E:128:CYS:SG	5:E:305:HOH:O	2.09	0.60
1:C:37:PHE:HD1	5:C:408:HOH:O	1.85	0.60
1:C:4:THR:HG23	1:C:6:PRO:HD2	1.83	0.60
1:C:33:GLN:OE1	1:C:37:PHE:HE2	1.83	0.59
1:B:73[B]:LYS:HE3	1:C:140[B]:VAL:HG23	1.84	0.59
1:E:21:GLN:HE22	1:E:24[B]:MET:CE	2.16	0.59
1:E:171:SER:C	4:E:204:HEZ:H62	2.23	0.59
1:E:79:VAL:HG23	1:E:81:GLN:HE22	1.67	0.59
1:F:33:GLN:CD	1:F:37:PHE:HE2	1.95	0.59
1:A:66:LYS:HD3	1:A:134:GLU:HG2	1.85	0.59
1:F:99[A]:LYS:NZ	1:F:99[A]:LYS:CB	2.66	0.58
1:A:113:LEU:O	1:A:117:LYS:HD3	2.04	0.58
1:A:33[B]:GLN:HG3	1:A:37:PHE:HE2	1.67	0.58
1:F:66:LYS:CD	1:F:134:GLU:HG2	2.32	0.58
1:E:142:ALA:CB	5:E:328:HOH:O	1.76	0.58
1:C:102:LEU:HA	1:C:146[B]:LEU:HD23	1.86	0.58
1:F:11:HIS:CE1	1:F:12:GLN:NE2	2.72	0.58
1:F:163:TRP:HH2	5:F:419:HOH:O	1.86	0.57
1:F:131[B]:LEU:HD22	1:F:136:LEU:HG	1.87	0.57
1:A:118:VAL:HG21	5:A:411:HOH:O	2.05	0.57
1:B:73[B]:LYS:HE3	1:C:140[B]:VAL:CG2	2.34	0.57
1:F:12:GLN:HE21	1:F:12:GLN:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:LEU:HD11	1:E:99[B]:LYS:CE	2.28	0.57
1:F:98:MET:SD	1:F:146[B]:LEU:HD13	2.45	0.57
1:A:127:MET:O	1:A:131[A]:LEU:HG	2.05	0.56
1:A:47:LYS:C	1:A:170:LEU:HD21	2.26	0.56
1:A:16:ALA:O	1:A:20:LYS:HE2	2.06	0.56
1:A:160:LEU:HD11	1:A:164:HIS:NE2	2.20	0.56
1:F:88[B]:ARG:NH1	1:F:91:TRP:CE3	2.74	0.56
1:B:146[B]:LEU:HD12	1:B:146[B]:LEU:O	2.06	0.56
1:B:154:ASN:ND2	5:B:302:HOH:O	2.18	0.55
1:A:164:HIS:CE1	1:C:164:HIS:CD2	2.94	0.55
1:A:167:GLN:HA	1:A:170:LEU:HD12	1.87	0.55
1:A:88[B]:ARG:NH2	5:A:309:HOH:O	2.40	0.55
1:F:102:LEU:HB2	1:F:146[B]:LEU:HD21	1.89	0.55
1:E:116:HIS:HB2	1:E:131[B]:LEU:CD2	2.36	0.55
1:B:52:PHE:HE1	1:B:149:ARG:NH1	2.05	0.55
1:B:131[B]:LEU:C	1:B:131[B]:LEU:HD12	2.27	0.55
1:D:13:ASP:CG	5:D:303:HOH:O	2.43	0.55
1:A:99[A]:LYS:HE2	5:A:400:HOH:O	2.06	0.55
1:E:37:PHE:CE1	5:E:414:HOH:O	2.60	0.55
1:E:33[B]:GLN:OE1	1:E:37:PHE:HE2	1.90	0.54
1:F:149:ARG:HG2	1:F:149:ARG:NH1	2.15	0.54
1:C:171:SER:C	4:C:203:HEZ:C3	2.76	0.54
1:F:102:LEU:CA	1:F:146[B]:LEU:HD23	2.32	0.54
1:A:101:ALA:HB3	1:A:146[B]:LEU:HD11	1.89	0.54
1:E:118:VAL:HG21	5:E:407:HOH:O	2.06	0.54
1:A:19:ASN:ND2	1:A:79:VAL:HG22	2.23	0.54
1:B:131[B]:LEU:HD12	1:B:131[B]:LEU:O	2.07	0.54
1:D:112:LEU:O	1:D:131[B]:LEU:HD21	2.08	0.54
1:A:123:GLY:CA	5:A:384:HOH:O	2.49	0.54
1:F:48:GLY:CA	1:F:170:LEU:HD22	2.19	0.54
1:F:88[A]:ARG:CZ	1:F:88[A]:ARG:CB	2.86	0.54
1:E:21:GLN:HE22	1:E:24[B]:MET:HE1	1.73	0.54
1:D:85[A]:LYS:HG2	1:F:82:PRO:HD3	1.88	0.54
1:B:69:LYS:O	1:B:73[A]:LYS:HG3	2.08	0.53
1:F:66:LYS:HD3	1:F:134:GLU:CG	2.38	0.53
1:D:131[B]:LEU:C	1:D:131[B]:LEU:HD12	2.27	0.53
1:A:48:GLY:HA2	1:A:170:LEU:HD23	1.90	0.53
1:F:81:GLN:CG	5:F:387:HOH:O	2.57	0.53
1:C:20[A]:LYS:NZ	5:C:303:HOH:O	2.41	0.53
1:C:158:LYS:N	1:C:158:LYS:CE	2.71	0.53
1:D:158:LYS:CD	1:D:158:LYS:N	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:GLN:HG3	5:E:401:HOH:O	2.08	0.53
1:A:48:GLY:HA2	1:A:170:LEU:CD2	2.38	0.53
1:B:48:GLY:CA	1:B:170:LEU:HG	2.39	0.52
1:B:48:GLY:HA2	1:B:170:LEU:HG	1.91	0.52
1:E:85:LYS:HE3	1:E:86:PRO:O	2.09	0.52
1:A:81[B]:GLN:NE2	5:A:310:HOH:O	2.40	0.52
1:D:96:ASP:OD1	5:D:301:HOH:O	2.18	0.52
1:B:98:MET:O	1:B:146[B]:LEU:HD11	2.09	0.52
1:E:98:MET:O	1:E:146[B]:LEU:HD11	2.08	0.52
1:A:82:PRO:HD3	1:B:85:LYS:HG2	1.89	0.52
1:D:35:MET:HE3	1:D:53:PHE:CZ	2.44	0.52
1:A:33[B]:GLN:CG	1:A:37:PHE:HE2	2.23	0.51
1:D:85[A]:LYS:H	1:F:82:PRO:HG3	1.74	0.51
1:F:95:LEU:HD11	1:F:99[B]:LYS:HE3	1.91	0.51
1:E:33[B]:GLN:OE1	1:E:37:PHE:CE2	2.63	0.51
1:A:82:PRO:HG3	1:B:85:LYS:H	1.74	0.51
1:F:149:ARG:HD3	5:F:415:HOH:O	2.11	0.51
1:A:101:ALA:HB3	1:A:146[B]:LEU:CD1	2.41	0.51
1:C:51[A]:LYS:NZ	5:C:304:HOH:O	2.44	0.51
4:B:203:HEZ:C2	5:B:417:HOH:O	2.59	0.51
1:D:102:LEU:HB2	1:D:146[B]:LEU:HD22	1.93	0.51
1:E:134:GLU:HB3	1:E:135:TYR:CE2	2.46	0.51
1:A:88[A]:ARG:CD	1:F:11:HIS:HE2	2.24	0.51
1:A:85[A]:LYS:H	1:B:82:PRO:HG3	1.76	0.51
1:D:160:LEU:HD11	1:D:164:HIS:NE2	2.25	0.51
1:B:118:VAL:HG21	5:B:394:HOH:O	2.10	0.50
1:F:47:LYS:C	1:F:170:LEU:HD21	2.32	0.50
1:A:73[A]:LYS:HG3	5:A:424:HOH:O	2.12	0.50
1:B:123:GLY:CA	5:B:360:HOH:O	2.55	0.50
1:B:134:GLU:HB3	1:B:135:TYR:CD2	2.47	0.50
1:B:52:PHE:CE1	1:B:149:ARG:NH1	2.79	0.50
1:D:118:VAL:HG21	5:D:387:HOH:O	2.11	0.50
1:B:102:LEU:HB2	1:B:146[B]:LEU:HG	1.94	0.50
1:E:85:LYS:CE	1:E:86:PRO:O	2.60	0.50
1:B:66:LYS:HD3	1:B:134:GLU:HG2	1.93	0.50
1:C:146[B]:LEU:C	1:C:146[B]:LEU:HD12	2.31	0.49
1:F:98:MET:SD	1:F:146[B]:LEU:CD1	3.01	0.49
1:F:85:LYS:HE2	1:F:86:PRO:O	2.11	0.49
1:A:79:VAL:HG23	1:A:81[A]:GLN:NE2	2.27	0.49
1:F:163:TRP:C	1:F:163:TRP:CD1	2.84	0.49
1:C:116:HIS:HB2	1:C:131[B]:LEU:HD23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:HD11	1:D:99[A]:LYS:HE2	1.95	0.49
1:E:114[A]:GLU:O	1:E:118:VAL:HG23	2.13	0.49
1:F:170:LEU:HD23	5:F:328:HOH:O	2.12	0.49
1:D:114[B]:GLU:O	1:D:118:VAL:HG23	2.12	0.49
1:C:167:GLN:HA	1:C:170:LEU:HD12	1.94	0.49
1:D:146[B]:LEU:HD23	1:D:146[B]:LEU:O	2.12	0.49
1:E:114[B]:GLU:OE1	1:E:114[B]:GLU:HA	2.11	0.49
1:A:81[A]:GLN:NE2	5:A:313:HOH:O	2.45	0.49
1:B:114[A]:GLU:O	1:B:118:VAL:HG23	2.13	0.49
1:D:85[B]:LYS:HE2	1:D:86:PRO:O	2.12	0.49
1:A:102:LEU:HB2	1:A:146[B]:LEU:CD2	2.43	0.48
1:B:114[B]:GLU:O	1:B:118:VAL:HG23	2.13	0.48
1:E:48:GLY:CA	1:E:170:LEU:HG	2.43	0.48
1:F:82:PRO:HD3	5:F:392:HOH:O	1.82	0.48
1:A:24[B]:MET:HE2	5:A:366:HOH:O	2.13	0.48
1:D:32:TYR:HD1	1:D:35:MET:HE2	1.79	0.48
1:C:95:LEU:HD11	1:C:99[A]:LYS:HE3	1.95	0.48
1:A:82:PRO:HD3	1:B:85:LYS:CG	2.44	0.48
1:E:146[B]:LEU:HD13	1:E:146[B]:LEU:O	2.14	0.48
1:F:102:LEU:CB	1:F:146[B]:LEU:HD21	2.43	0.48
1:A:163:TRP:CZ3	1:C:168:LYS:HE3	2.49	0.48
1:F:88[B]:ARG:NH1	1:F:91:TRP:CZ3	2.82	0.48
1:F:131[B]:LEU:CD2	1:F:136:LEU:HG	2.44	0.48
1:C:4:THR:HG21	1:C:75:GLY:CA	2.44	0.47
1:F:149:ARG:CD	5:F:415:HOH:O	2.61	0.47
1:C:171:SER:C	4:C:203:HEZ:H31	2.35	0.47
1:D:35:MET:CE	1:D:53:PHE:CD1	2.97	0.47
1:D:88[B]:ARG:N	1:D:88[B]:ARG:HD2	2.29	0.47
1:F:99[A]:LYS:HB2	1:F:99[A]:LYS:HZ3	1.78	0.47
1:B:19:ASN:ND2	1:B:79:VAL:HG22	2.29	0.47
1:D:142:ALA:O	1:D:146[B]:LEU:HB2	2.13	0.47
1:C:102:LEU:CA	1:C:146[B]:LEU:CD2	2.92	0.47
1:D:85[B]:LYS:H	1:F:82:PRO:HG3	1.78	0.47
1:E:146[B]:LEU:CD1	1:E:146[B]:LEU:C	2.82	0.47
1:F:98:MET:O	1:F:146[B]:LEU:HD11	2.15	0.47
4:D:203:HEZ:H52	5:D:433:HOH:O	2.14	0.47
1:F:116:HIS:HB2	1:F:131[B]:LEU:CD1	2.44	0.47
1:A:102:LEU:HB2	1:A:146[B]:LEU:HD22	1.97	0.47
1:D:116:HIS:HB2	1:D:131[B]:LEU:HD23	1.95	0.47
1:C:70:TYR:HA	1:C:73[A]:LYS:HE3	1.98	0.46
1:C:82:PRO:CD	1:E:85:LYS:HG2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:GLN:NE2	1:E:24[B]:MET:HE2	2.28	0.46
1:B:66:LYS:HD3	1:B:134:GLU:CG	2.46	0.46
1:C:131[B]:LEU:CD1	1:C:131[B]:LEU:C	2.67	0.46
1:C:63[B]:HIS:CD2	5:C:309:HOH:O	2.68	0.46
1:D:48:GLY:CA	1:D:170:LEU:HG	2.46	0.46
1:C:37:PHE:CE1	5:C:408:HOH:O	2.67	0.46
1:D:134:GLU:HB3	1:D:135:TYR:CE2	2.50	0.46
1:F:102:LEU:HB2	1:F:146[B]:LEU:CD2	2.45	0.46
1:C:102:LEU:H	1:C:146[B]:LEU:HD21	1.76	0.46
1:F:33:GLN:HE21	4:F:204:HEZ:C1	2.29	0.46
1:B:20:LYS:CE	5:B:393:HOH:O	2.48	0.46
1:C:4:THR:CG2	1:C:7:ARG:HB2	2.45	0.46
1:A:158:LYS:CD	1:A:158:LYS:N	2.67	0.45
1:C:131[B]:LEU:CD1	1:C:135:TYR:HB2	2.46	0.45
1:E:114[B]:GLU:OE1	1:E:114[B]:GLU:CA	2.65	0.45
1:C:118:VAL:HG21	5:C:416:HOH:O	2.16	0.45
1:D:70:TYR:HA	1:D:73[A]:LYS:HE3	1.99	0.45
1:E:19:ASN:ND2	1:E:79:VAL:HG22	2.32	0.45
1:B:146[B]:LEU:HD12	1:B:146[B]:LEU:C	2.36	0.45
1:E:149:ARG:CG	1:E:149:ARG:NH1	2.34	0.45
1:F:131[B]:LEU:HA	1:F:131[B]:LEU:HD23	1.66	0.45
1:A:131[B]:LEU:HD12	1:A:135:TYR:HB2	1.98	0.45
1:B:102:LEU:N	1:B:146[B]:LEU:HD21	2.31	0.45
1:E:69:LYS:HG2	1:E:73[A]:LYS:CE	2.47	0.45
1:C:66:LYS:HD3	1:C:134:GLU:CG	2.43	0.45
1:E:149:ARG:HD3	5:E:420:HOH:O	2.17	0.45
1:D:35:MET:HE1	1:D:53:PHE:CE1	2.52	0.45
1:F:123:GLY:CA	5:F:407:HOH:O	2.56	0.45
1:A:134:GLU:HB3	1:A:135:TYR:CD2	2.52	0.44
1:F:131[B]:LEU:HD22	1:F:132:GLU:N	2.25	0.44
1:D:69:LYS:HG2	1:D:73[A]:LYS:CE	2.47	0.44
1:D:163:TRP:HZ2	5:D:409:HOH:O	1.99	0.44
1:E:69:LYS:HG2	1:E:73[A]:LYS:HE2	1.99	0.44
1:D:146[B]:LEU:C	1:D:146[B]:LEU:HD23	2.37	0.44
1:F:134:GLU:HB3	1:F:135:TYR:CD2	2.52	0.44
1:A:163:TRP:CZ3	1:C:168:LYS:CE	3.01	0.44
1:A:85[B]:LYS:H	1:B:82:PRO:HG3	1.82	0.44
1:B:145:ASP:CG	1:B:149:ARG:NH1	2.71	0.44
1:D:67:LEU:HG	1:D:135:TYR:OH	2.18	0.44
1:F:88[A]:ARG:HG3	1:F:91:TRP:CE3	2.52	0.44
1:F:102:LEU:H	1:F:146[B]:LEU:HD21	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LYS:HB3	1:C:170:LEU:HD21	1.98	0.44
1:F:4:THR:CG2	1:F:7:ARG:HB2	2.47	0.44
1:E:24[B]:MET:HE1	1:E:111:SER:HB3	2.00	0.43
1:C:4:THR:OG1	1:C:77:ARG:NH2	2.52	0.43
1:C:69:LYS:HG2	1:C:73[A]:LYS:HE2	1.99	0.43
1:A:33[A]:GLN:CD	1:A:37:PHE:CE2	2.56	0.43
1:E:116:HIS:CB	1:E:131[B]:LEU:HD23	2.48	0.43
1:F:88[A]:ARG:CG	1:F:91:TRP:CZ3	3.01	0.43
1:D:167:GLN:HA	1:D:170:LEU:HD12	2.01	0.43
1:F:66:LYS:CD	1:F:134:GLU:CG	2.97	0.43
1:C:47:LYS:CB	1:C:170:LEU:HD21	2.49	0.43
1:F:4:THR:HG22	1:F:7:ARG:HB2	2.01	0.42
1:C:102:LEU:CA	1:C:146[B]:LEU:HD21	2.49	0.42
1:D:47:LYS:CB	1:D:170:LEU:HD21	2.49	0.42
1:A:66:LYS:HD3	1:A:134:GLU:CG	2.48	0.42
1:B:95:LEU:O	1:B:99[B]:LYS:HG3	2.20	0.42
1:F:164:HIS:CD2	1:F:168:LYS:HE3	2.55	0.42
1:B:131[B]:LEU:HD12	1:B:136:LEU:HG	2.01	0.42
1:C:85:LYS:HE2	1:C:86:PRO:O	2.19	0.42
1:E:72:ASN:ND2	5:E:309:HOH:O	2.53	0.42
1:C:14:SER:O	1:C:18:ILE:HG23	2.20	0.42
1:F:114:GLU:O	1:F:118:VAL:HG23	2.20	0.42
1:C:48:GLY:CA	1:C:170:LEU:HG	2.50	0.42
1:F:163:TRP:CD1	1:F:164:HIS:N	2.88	0.42
1:B:82:PRO:CD	5:B:391:HOH:O	2.02	0.41
1:E:4:THR:CG2	5:E:410:HOH:O	2.68	0.41
1:D:114[A]:GLU:OE1	1:D:114[A]:GLU:HA	2.20	0.41
1:E:149:ARG:CD	5:E:420:HOH:O	2.68	0.41
1:A:48:GLY:CA	1:A:170:LEU:CD2	2.97	0.41
1:E:51:LYS:HE3	1:E:170:LEU:HD23	2.02	0.41
1:C:85:LYS:H	1:E:82:PRO:HG3	1.85	0.41
1:A:98:MET:O	1:A:146[B]:LEU:HD11	2.20	0.41
1:B:66:LYS:CD	1:B:134:GLU:HG2	2.51	0.41
1:D:12:GLN:HG3	5:D:365:HOH:O	2.20	0.41
1:A:107:SER:HB3	5:A:435:HOH:O	2.20	0.41
1:C:116:HIS:HB2	1:C:131[B]:LEU:CD2	2.50	0.41
1:C:112:LEU:O	1:C:131[B]:LEU:HD21	2.20	0.41
1:F:12:GLN:N	1:F:12:GLN:HE21	2.17	0.41
1:C:142:ALA:O	1:C:146[A]:LEU:HG	2.21	0.41
4:C:203:HEZ:C6	5:C:377:HOH:O	2.68	0.41
1:D:35:MET:HE3	1:D:53:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:HIS:CB	1:A:131[B]:LEU:CD2	2.71	0.41
4:B:203:HEZ:C3	5:B:417:HOH:O	2.69	0.41
1:C:4:THR:HG21	1:C:75:GLY:HA3	2.02	0.41
1:A:51:LYS:HE3	1:A:170:LEU:HD23	1.93	0.41
1:A:88[A]:ARG:HD3	1:F:11:HIS:HE2	1.86	0.41
1:D:4:THR:HG22	1:D:7:ARG:HB2	2.03	0.41
1:A:146[B]:LEU:HD21	1:A:150:ILE:HD11	2.03	0.40
1:D:96:ASP:HA	1:D:99[B]:LYS:NZ	2.37	0.40
1:E:70:TYR:HA	1:E:73[A]:LYS:HE3	2.04	0.40
1:F:134:GLU:HB3	1:F:135:TYR:CE2	2.56	0.40
1:C:131[B]:LEU:HD11	1:C:136:LEU:CD2	2.50	0.40
1:D:117:LYS:NZ	5:D:312:HOH:O	2.54	0.40
1:D:4:THR:HG21	1:D:75:GLY:CA	2.51	0.40
1:F:88[A]:ARG:HG2	1:F:91:TRP:CZ3	2.57	0.40
1:A:154:ASN:ND2	5:A:305:HOH:O	2.17	0.40
1:E:158:LYS:H	1:E:158:LYS:HG2	1.51	0.40
1:E:88[A]:ARG:NE	1:E:88[A]:ARG:HA	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:437:HOH:O	5:E:416:HOH:O[4_565]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	181/171 (106%)	179 (99%)	2 (1%)	0	100	100
1	B	182/171 (106%)	180 (99%)	2 (1%)	0	100	100
1	C	181/171 (106%)	179 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	183/171 (107%)	181 (99%)	2 (1%)	0	100	100
1	E	183/171 (107%)	181 (99%)	2 (1%)	0	100	100
1	F	177/171 (104%)	175 (99%)	2 (1%)	0	100	100
All	All	1087/1026 (106%)	1075 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	158/148 (107%)	147 (93%)	11 (7%)	15	6
1	B	158/148 (107%)	149 (94%)	9 (6%)	20	9
1	C	159/148 (107%)	150 (94%)	9 (6%)	20	9
1	D	160/148 (108%)	149 (93%)	11 (7%)	15	6
1	E	161/148 (109%)	149 (92%)	12 (8%)	13	4
1	F	147/148 (99%)	127 (86%)	20 (14%)	3	1
All	All	943/888 (106%)	871 (92%)	72 (8%)	14	4

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	40	ASP
1	A	82	PRO
1	A	85[A]	LYS
1	A	85[B]	LYS
1	A	107	SER
1	A	114	GLU
1	A	134	GLU
1	A	139	GLN
1	A	149	ARG

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Mol	Chain	Res	Type
1	A	158	LYS
1	B	30	TYR
1	B	40[A]	ASP
1	B	40[B]	ASP
1	B	69	LYS
1	B	82	PRO
1	B	87	ASP
1	B	134	GLU
1	B	158	LYS
1	B	164	HIS
1	C	24	MET
1	C	40	ASP
1	C	81	GLN
1	C	82	PRO
1	C	85	LYS
1	C	114	GLU
1	C	158	LYS
1	C	168	LYS
1	C	171	SER
1	D	5	MET
1	D	24	MET
1	D	30	TYR
1	D	33[A]	GLN
1	D	33[B]	GLN
1	D	82	PRO
1	D	114[A]	GLU
1	D	114[B]	GLU
1	D	134	GLU
1	D	158	LYS
1	D	168	LYS
1	E	5	MET
1	E	12[A]	GLN
1	E	12[B]	GLN
1	E	30	TYR
1	E	56	SER
1	E	82	PRO
1	E	99[A]	LYS
1	E	99[B]	LYS
1	E	134	GLU
1	E	149	ARG
1	E	158	LYS
1	E	168	LYS

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Mol	Chain	Res	Type
1	F	12	GLN
1	F	20	LYS
1	F	30	TYR
1	F	40	ASP
1	F	51	LYS
1	F	82	PRO
1	F	85	LYS
1	F	88[A]	ARG
1	F	88[B]	ARG
1	F	99[A]	LYS
1	F	99[B]	LYS
1	F	114	GLU
1	F	134	GLU
1	F	146[A]	LEU
1	F	146[B]	LEU
1	F	149	ARG
1	F	163	TRP
1	F	164	HIS
1	F	168	LYS
1	F	170	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	B	23	ASN
1	B	81	GLN
1	C	164	HIS
1	D	81	GLN
1	E	21	GLN
1	E	72	ASN
1	E	81	GLN
1	F	12	GLN
1	F	33	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 14 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HEZ	E	204	-	7,7,7	0.28	0	6,6,6	0.88	0
4	HEZ	F	205	-	7,7,7	0.45	0	6,6,6	0.55	0
4	HEZ	F	204	-	7,7,7	0.25	0	6,6,6	0.49	0
4	HEZ	D	203	-	7,7,7	0.35	0	6,6,6	0.74	0
4	HEZ	B	203	-	7,7,7	0.40	0	6,6,6	0.64	0
4	HEZ	E	203	-	7,7,7	0.52	0	6,6,6	0.45	0
4	HEZ	C	203	-	7,7,7	0.46	0	6,6,6	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEZ	E	204	-	-	4/5/5/5	-
4	HEZ	F	205	-	-	2/5/5/5	-
4	HEZ	F	204	-	-	3/5/5/5	-
4	HEZ	D	203	-	-	4/5/5/5	-
4	HEZ	B	203	-	-	2/5/5/5	-
4	HEZ	E	203	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEZ	C	203	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	203	HEZ	C2-C3-C4-C5
4	B	203	HEZ	C1-C2-C3-C4
4	F	204	HEZ	C2-C3-C4-C5
4	D	203	HEZ	C1-C2-C3-C4
4	E	203	HEZ	C1-C2-C3-C4
4	E	203	HEZ	C4-C5-C6-O6
4	C	203	HEZ	O1-C1-C2-C3
4	F	204	HEZ	O1-C1-C2-C3
4	C	203	HEZ	C4-C5-C6-O6
4	B	203	HEZ	C3-C4-C5-C6
4	F	205	HEZ	C4-C5-C6-O6
4	D	203	HEZ	C3-C4-C5-C6
4	E	204	HEZ	C2-C3-C4-C5
4	E	204	HEZ	C3-C4-C5-C6
4	E	204	HEZ	O1-C1-C2-C3
4	E	203	HEZ	O1-C1-C2-C3
4	F	204	HEZ	C4-C5-C6-O6
4	D	203	HEZ	C4-C5-C6-O6
4	D	203	HEZ	C2-C3-C4-C5
4	F	205	HEZ	C1-C2-C3-C4
4	E	204	HEZ	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	204	HEZ	3	0
4	F	205	HEZ	1	0
4	F	204	HEZ	1	0
4	D	203	HEZ	3	0
4	B	203	HEZ	4	0
4	C	203	HEZ	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	170/171 (99%)	0.25	7 (4%)	37 39	17, 22, 33, 59	5 (2%)
1	B	170/171 (99%)	0.10	4 (2%)	59 61	18, 23, 33, 59	3 (1%)
1	C	170/171 (99%)	0.25	10 (5%)	22 24	18, 22, 31, 65	10 (5%)
1	D	170/171 (99%)	0.25	6 (3%)	44 46	17, 22, 32, 62	8 (4%)
1	E	170/171 (99%)	0.22	7 (4%)	37 39	18, 22, 34, 61	7 (4%)
1	F	170/171 (99%)	0.12	5 (2%)	51 54	18, 21, 31, 52	7 (4%)
All	All	1020/1026 (99%)	0.20	39 (3%)	40 43	17, 22, 34, 65	40 (3%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ALA	6.9
1	A	2	ALA	4.5
1	E	37	PHE	4.1
1	F	2	ALA	3.9
1	D	3	GLU	3.8
1	E	2	ALA	3.6
1	A	131[A]	LEU	3.4
1	A	3	GLU	3.4
1	A	163	TRP	3.0
1	C	73[A]	LYS	3.0
1	D	37	PHE	3.0
1	C	146[A]	LEU	2.9
1	C	2	ALA	2.9
1	F	146[A]	LEU	2.8
1	F	88[A]	ARG	2.8
1	E	164	HIS	2.7
1	E	73[A]	LYS	2.7
1	C	82	PRO	2.7
1	E	163	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	12[A]	GLN	2.5
1	D	131[A]	LEU	2.5
1	C	164	HIS	2.4
1	C	4	THR	2.4
1	E	12[A]	GLN	2.4
1	A	4	THR	2.2
1	C	3	GLU	2.2
1	B	146[A]	LEU	2.2
1	C	163	TRP	2.2
1	A	146[A]	LEU	2.2
1	A	170	LEU	2.2
1	C	158	LYS	2.1
1	F	131[A]	LEU	2.1
1	F	163	TRP	2.1
1	B	3	GLU	2.1
1	C	79	VAL	2.1
1	B	37	PHE	2.1
1	D	163	TRP	2.1
1	E	131[A]	LEU	2.1
1	D	4	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FE2	A	201	1/1	0.70	0.39	104,104,104,104	0
4	HEZ	B	203	8/8	0.76	0.16	42,44,52,53	0
4	HEZ	C	203	8/8	0.77	0.20	43,50,52,53	0

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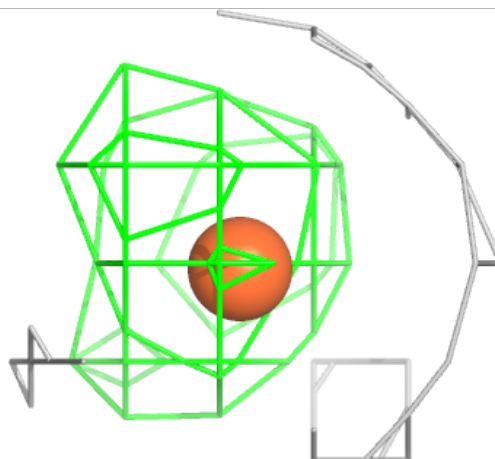
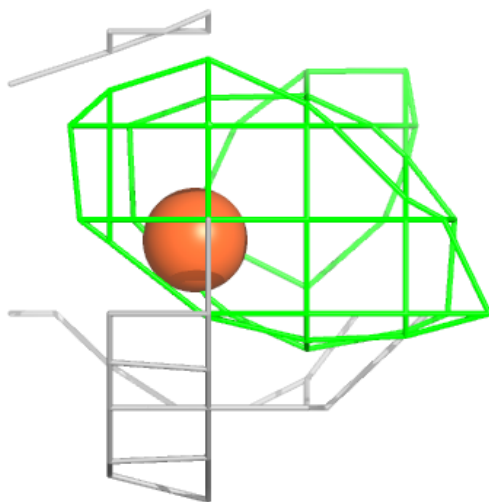
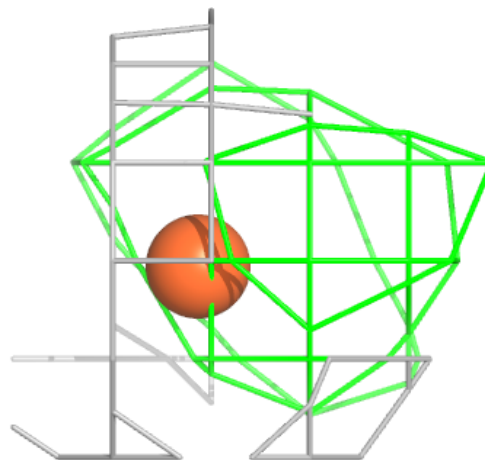
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	HEZ	D	203	8/8	0.78	0.20	40,44,50,59	0
4	HEZ	E	203	8/8	0.81	0.17	43,50,52,56	0
4	HEZ	F	204	8/8	0.85	0.23	40,46,55,63	0
4	HEZ	E	204	8/8	0.85	0.15	42,43,48,55	0
4	HEZ	F	205	8/8	0.85	0.14	35,44,47,52	0
3	FE	C	202	1/1	0.87	0.34	71,71,71,71	1
2	FE2	F	201	1/1	0.88	0.13	75,75,75,75	0
3	FE	A	203	1/1	0.91	0.55	68,68,68,68	1
3	FE	D	202	1/1	0.97	0.25	62,62,62,62	1
3	FE	B	201	1/1	0.98	0.04	27,27,27,27	1
3	FE	E	202	1/1	0.98	0.34	61,61,61,61	1
3	FE	B	202	1/1	0.98	0.26	48,48,48,48	1
3	FE	E	201	1/1	0.99	0.04	28,28,28,28	1
3	FE	C	201	1/1	0.99	0.04	25,25,25,25	1
3	FE	A	202	1/1	0.99	0.05	26,26,26,26	1
3	FE	F	203	1/1	0.99	0.27	54,54,54,54	1
3	FE	D	201	1/1	0.99	0.04	28,28,28,28	0
3	FE	F	202	1/1	1.00	0.04	26,26,26,26	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

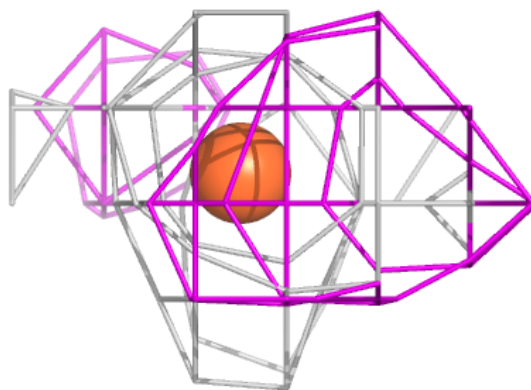
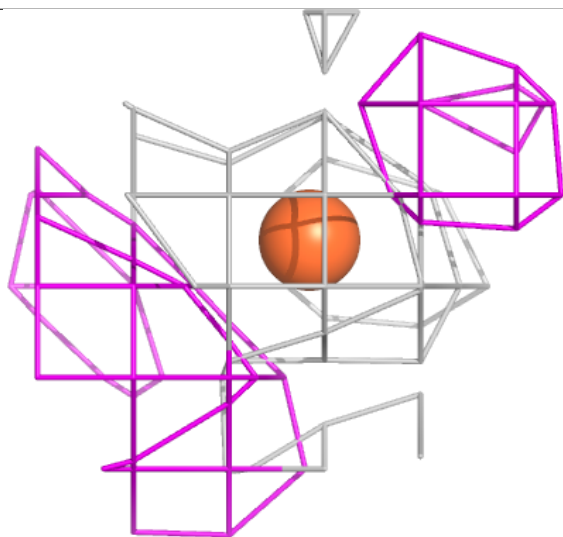
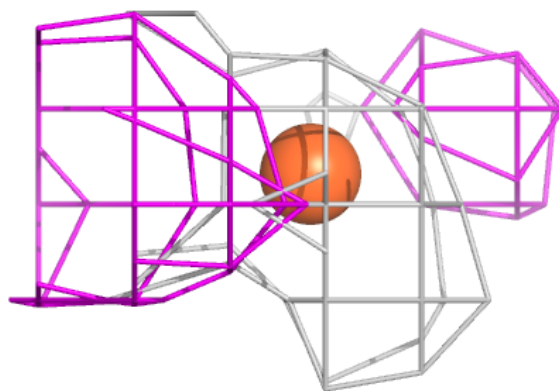
Electron density around FE2 A 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



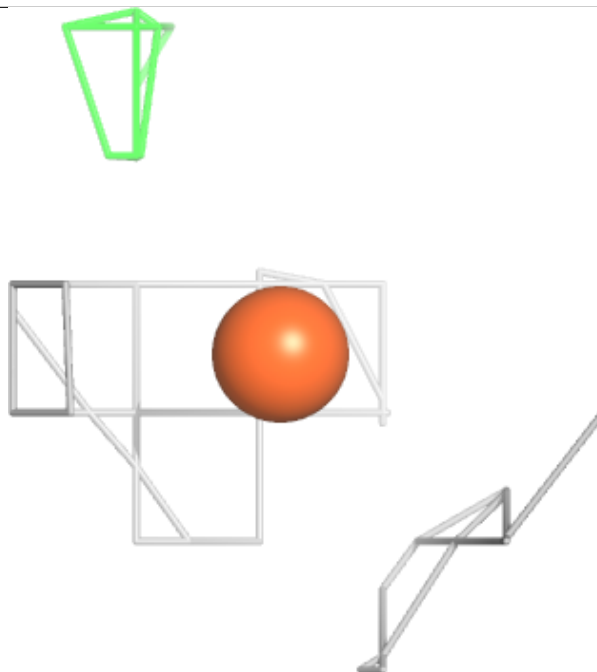
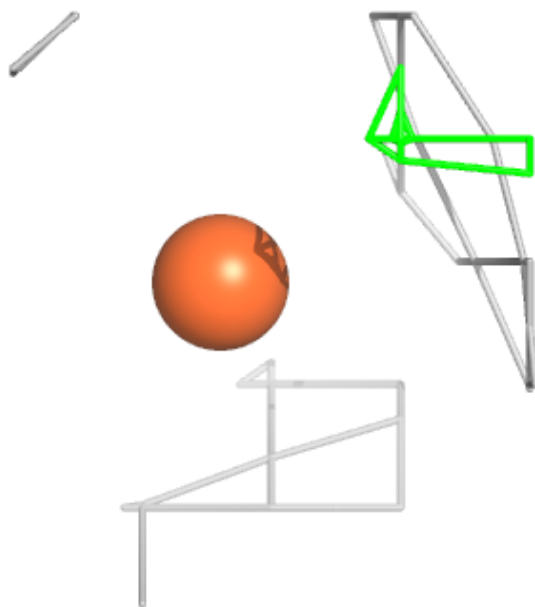
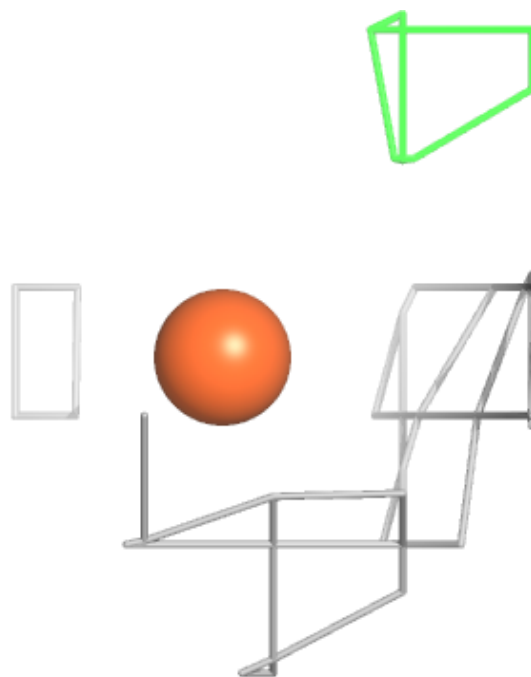
Electron density around FE C 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



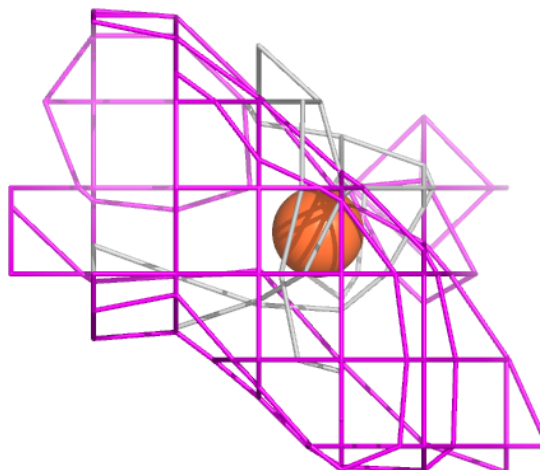
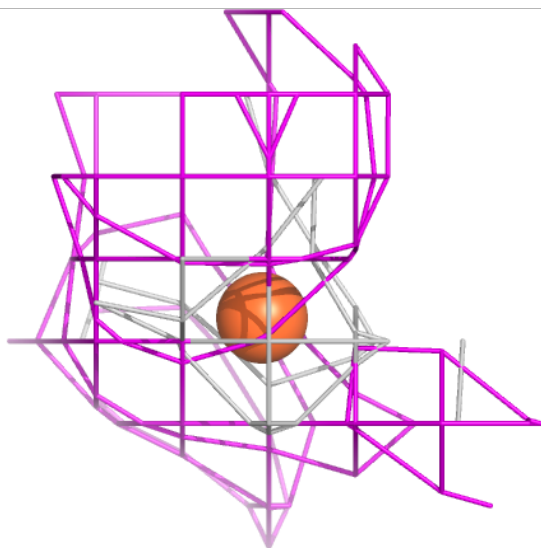
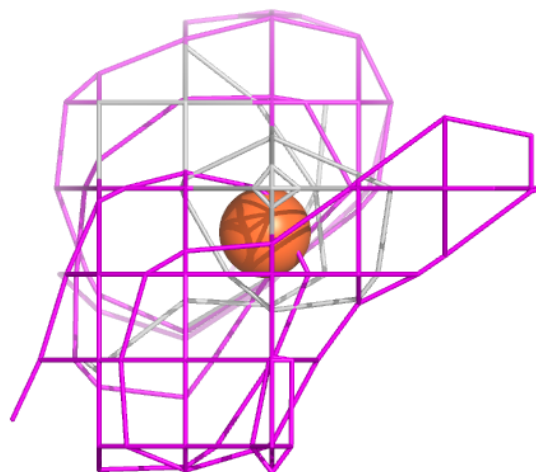
Electron density around FE2 F 201:

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 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



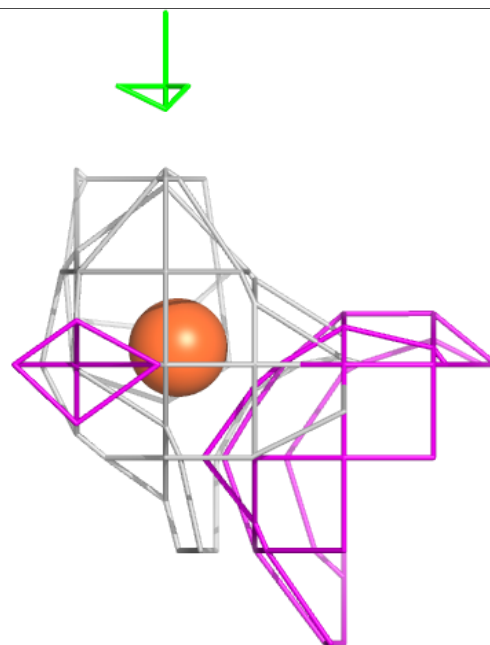
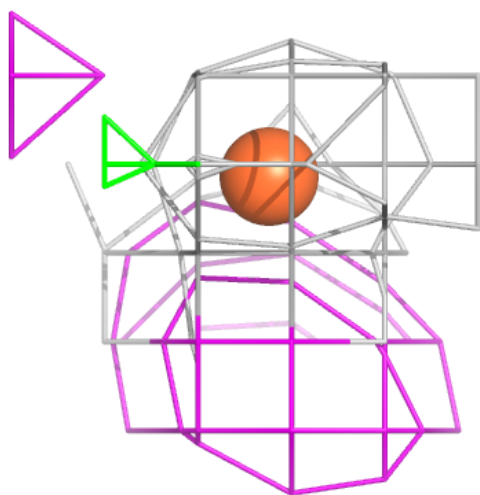
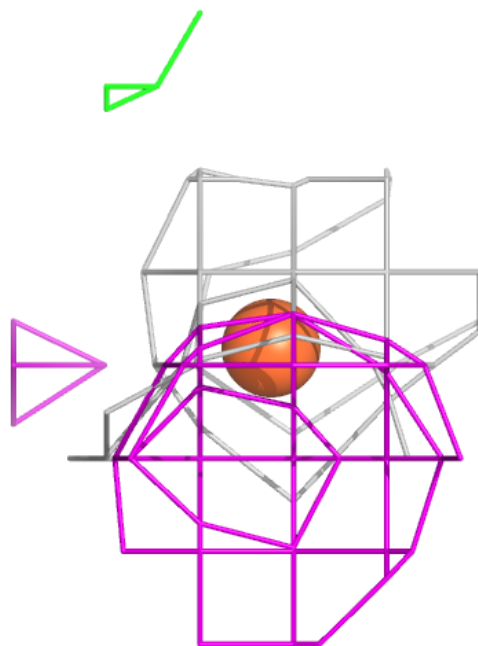
Electron density around FE A 203:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



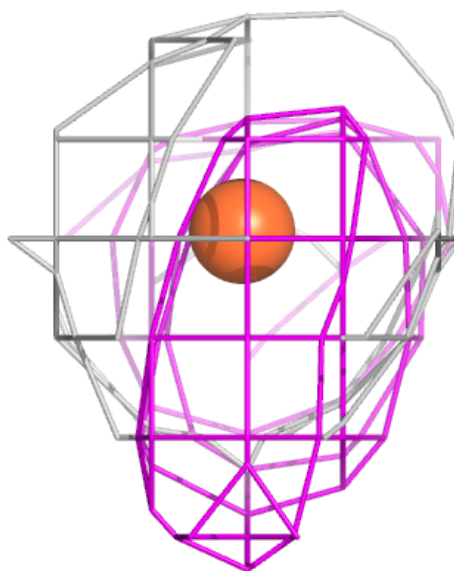
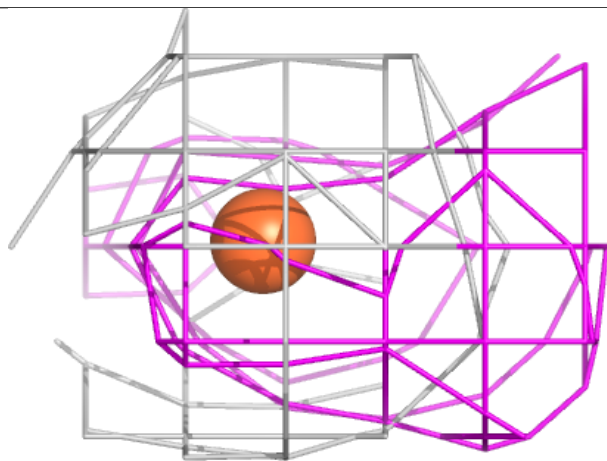
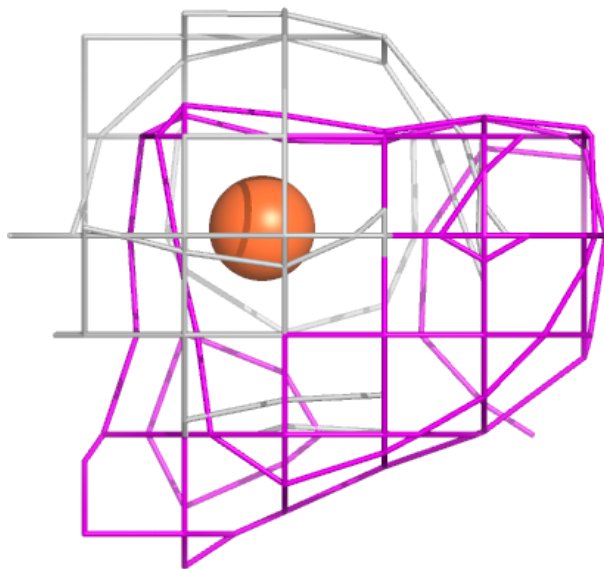
Electron density around FE D 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



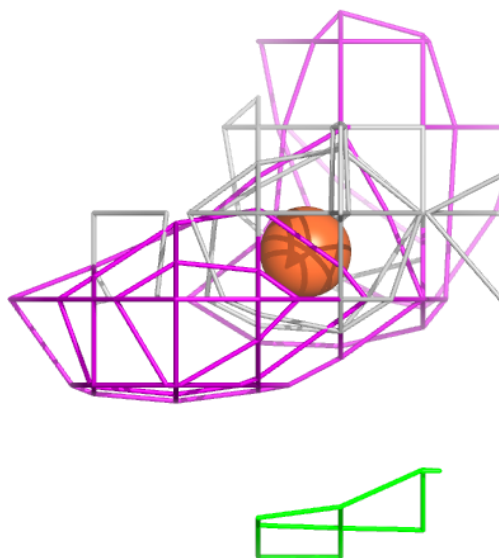
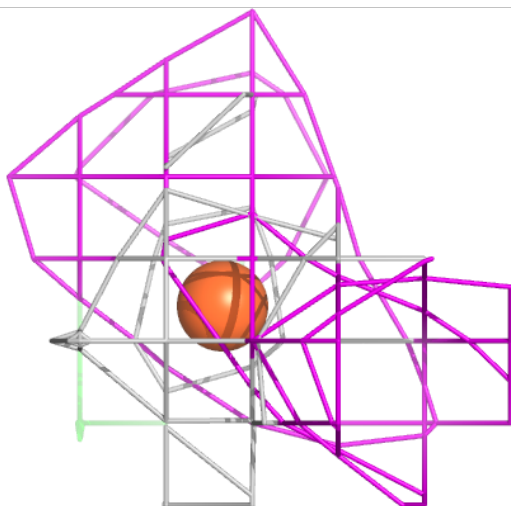
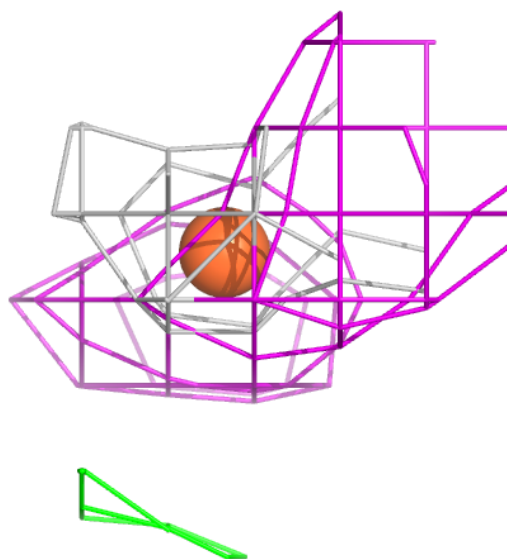
Electron density around FE B 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



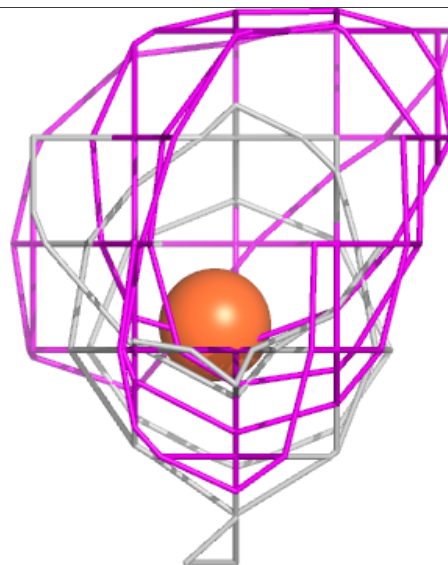
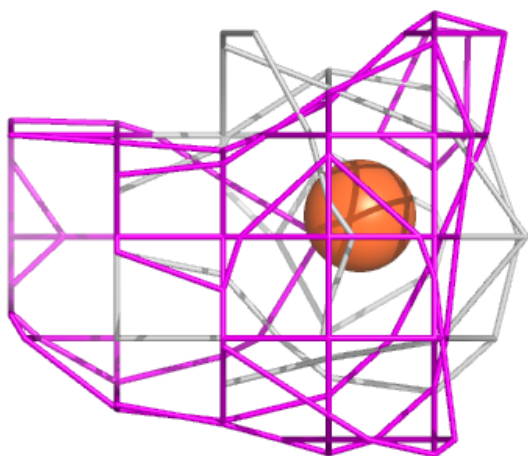
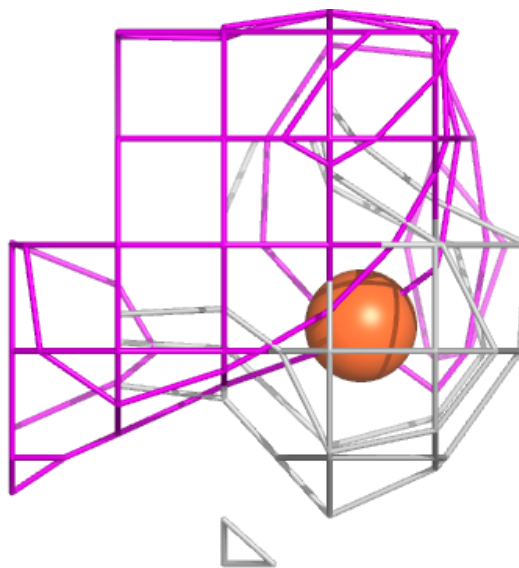
Electron density around FE E 202:

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and green (positive)



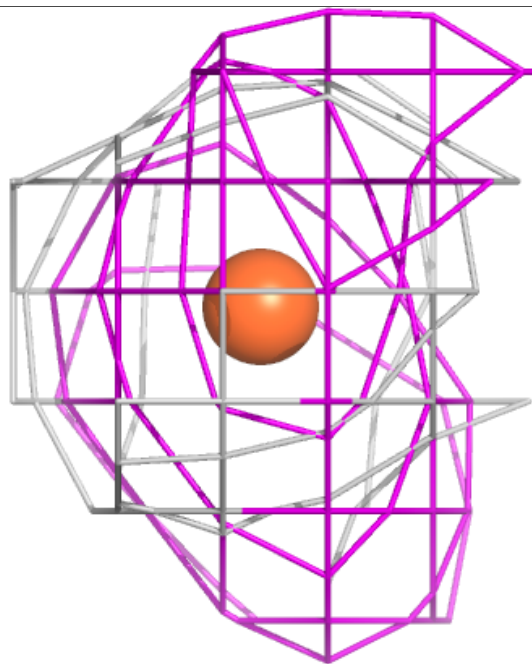
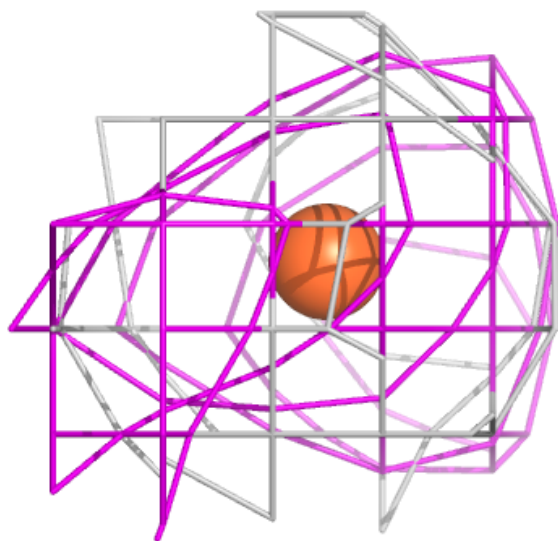
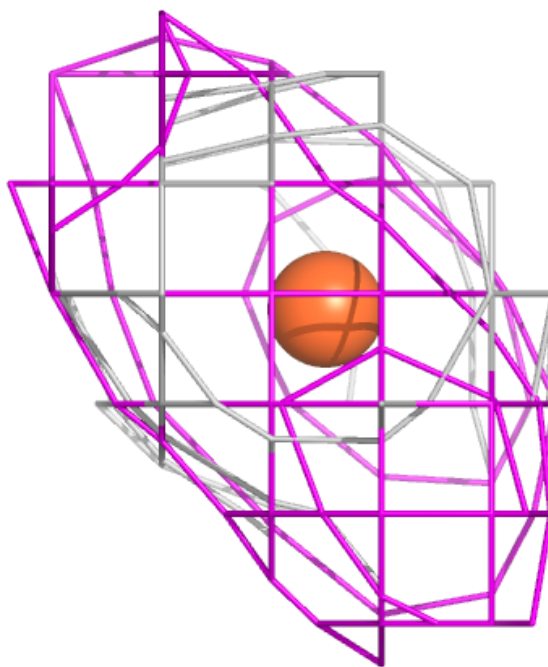
Electron density around FE B 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



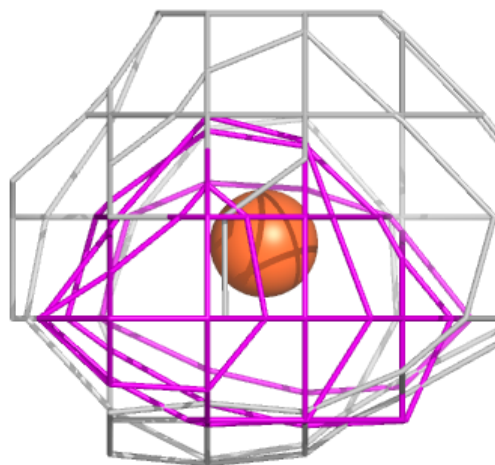
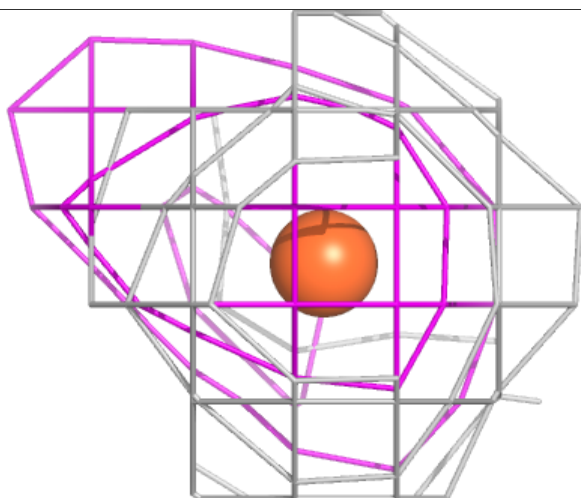
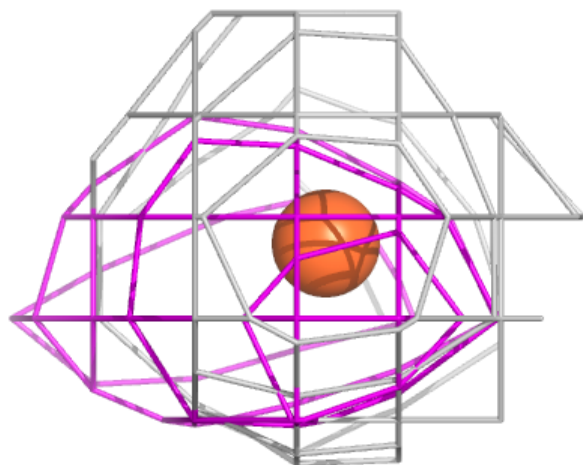
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and green (positive)



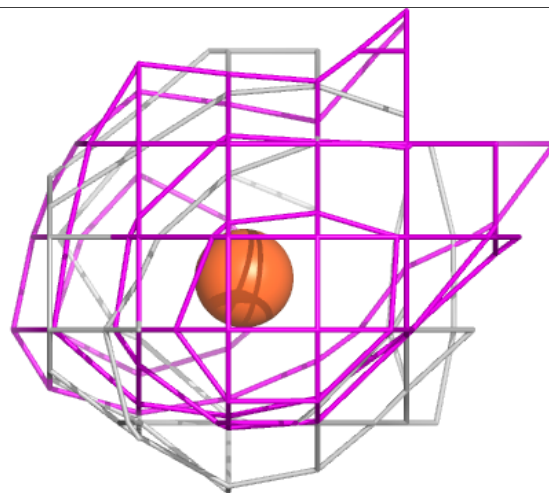
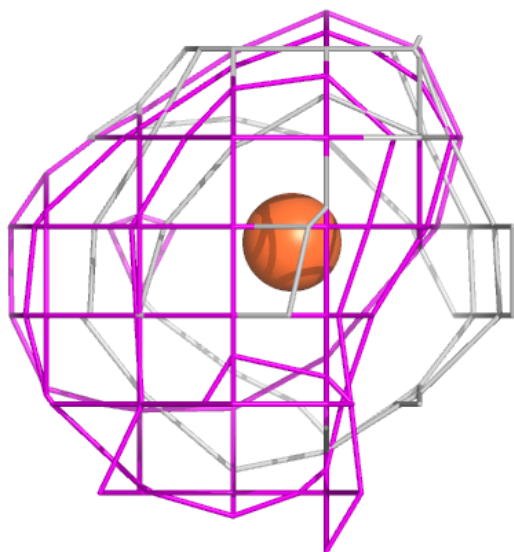
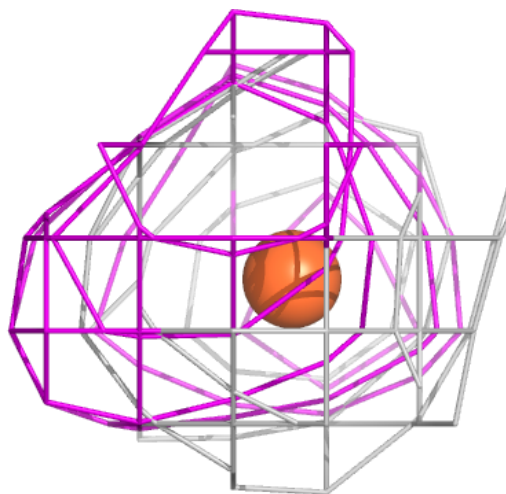
Electron density around FE C 201:

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and green (positive)



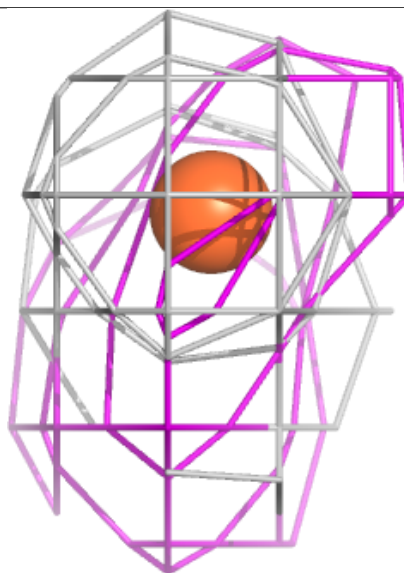
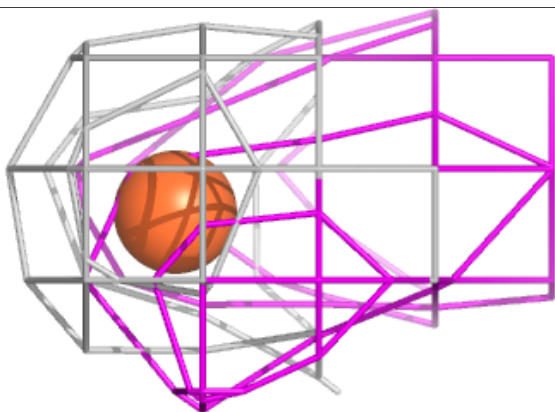
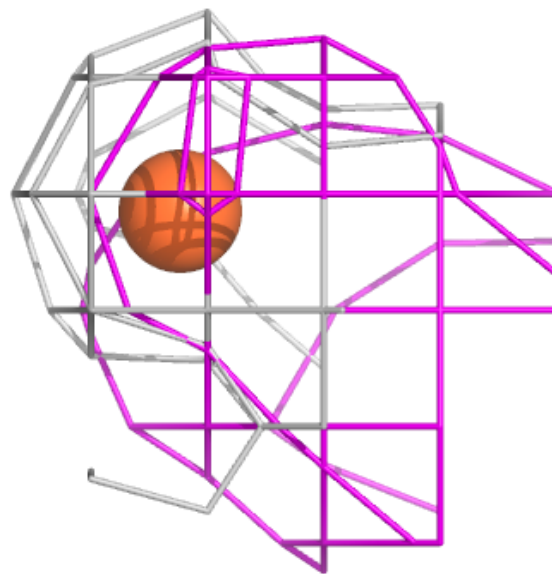
Electron density around FE A 202:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



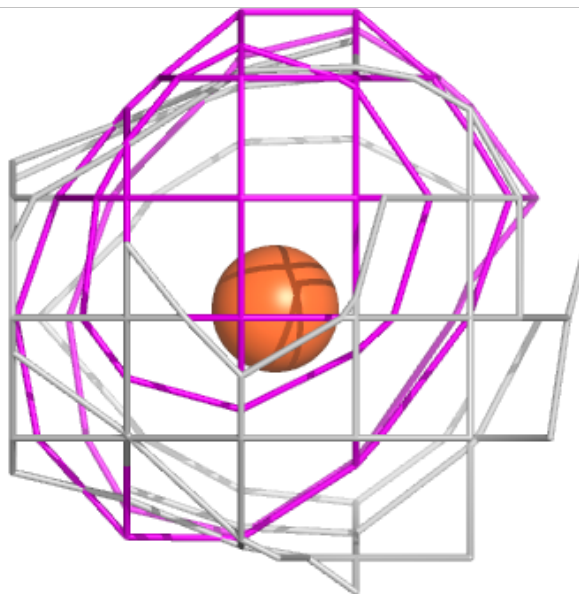
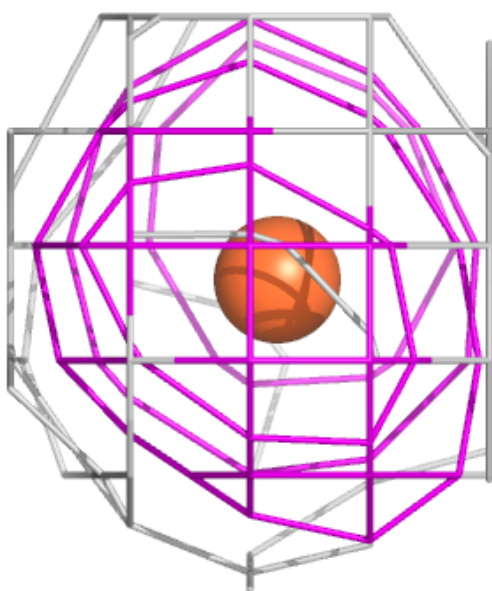
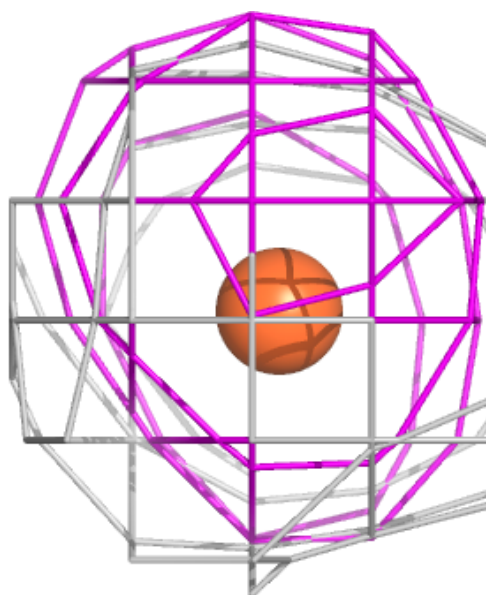
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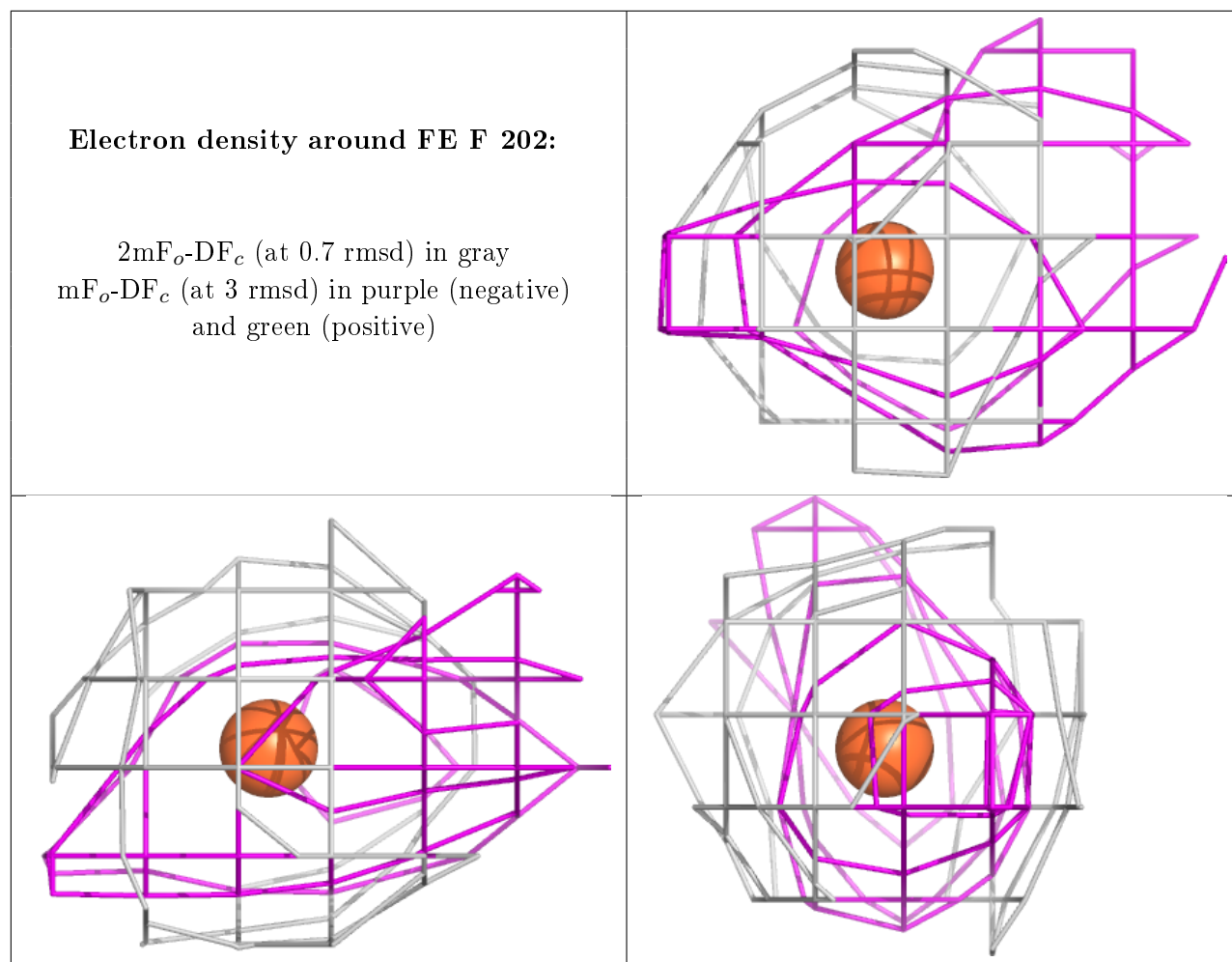
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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FE D 201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.